

Benzoic acid, 3-methoxy-
586-38-9 | DTXSID2060410

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 |

Model Results

Predicted value: 279 °C

Global applicability domain: Inside

Local applicability domain index: 6.93e-01

Confidence level: 8.67e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 4-methoxy-

Measured: 277

Predicted: 279

Image not found

Phenoxyacetic acid

Measured: 285

Predicted: 279

Image not found

Hydrocinnamic acid

Measured: 280

Predicted: 270

Image not found

Acetic acid, (p-tolyl)-

Measured: 265

Predicted: 270

Image not found

2-Chlorobenzoic acid

Measured: 287

Predicted: 273